

Representation and Construction of Main Effect Plans
in Terms of (0,1)-Matrices*

by D. A. Anderson** and W. T. Federer

Cornell University

Abstract

Let T denote a main effect plan for the s^n factorial with N assemblies, that is T is an $N \times n$ matrix with elements from the $\{0, 1, \dots, s-1\}$. Denote by T_0, T_1, \dots, T_{s-1} the $N \times n$ incidence matrices of $0, 1, \dots, s-1$ respectively, so that $T = \sum_i T_i$ and $\sum_i T_i = J(N \times n)$. Using the Helmert polynomials to define single degree of freedom main effect contrasts we write $E\{\underline{y}\} = X\underline{\beta}$, where X is the design matrix D corresponding to T . A transformation G is obtained for which $XG = X^* = [\underline{1} : T_1 : \dots : T_{s-1}]$ thus giving a representation for the design matrix directly in terms of the (0,1)-incidence matrices. It is shown that $|G| = (s!)^{-n}(-1)^{(s-1)n}$ and $|X'X| = (s!)^{2n}|X^*X^*|$. If T is a saturated main effect plan, then $|X| = (s!)^n|X^*|$. Thus the determinant of the information matrix is directly expressible in terms of the determinant of a (0,1)-matrix. These results are extended to include the general asymmetrical factorial $\Pi s_i^{n_i}$. It is shown that the one at a time main effect plan is 'least' optimal in terms of the determinant criteria. The representation of orthogonal main effect plans, the effect of collapsing levels in an orthogonal main effect plan, and the representation of sets of orthogonal $F(n, \lambda)$ squares are given. Other series of designs and methods of construction of main effect plans obtained from the representation are presented. An upper bound on $|X^*X^*|$ and on $|X'X|$ is presented; some possible values for these quantities are given also.

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1. Introduction. In a factorial treatment design, the design matrix D consists of a designation of the number of factors n and of the number of levels, s_i , for the i^{th} factor, $i = 1, 2, \dots, n$. The total number of combinations is $\prod_{i=1}^n s_i$. In the current literature, the design matrix D is almost universally replaced by a matrix X , which reflects the p single degree of freedom parametric contrasts in the parametric vector $\beta_{p \times 1}$ from the usual regression equation $E(y_{N \times 1}) = X_{N \times p} \beta_{p \times 1}$; then the normal equations are obtained as $X'X\beta = X'y$, and solutions for the parameters are found from the normal equations. The matrix $X'X$ is denoted as the information matrix and the generalized inverse $(X'X)^-$ is denoted as the variance-covariance matrix of estimable functions of the parameters in β . It should be noted here that the design matrix D , the vector of observations, and the parametric vector β provide all the available information from the experiment. The use of the X -matrix is merely a convenience. Therefore, if possible, it would be desirable to utilize the D matrix directly in place of the X matrix in the normal equations and in the variance-covariance matrix. Raktveit and Federer [1970] obtained such a representation for main effect plans from the 2^n factorial. Since there are only two levels, they used a (0,1)-matrix and demonstrated a direct relationship between D and X and between $D'D$ and $X'X$. In doing this they transformed the X matrix to an X^* matrix where $X^* = (\mathbf{1} D)$ and $\mathbf{1}$ is a column vector of ones. Thus, it was possible to provide a characterization of optimal saturated main effect plans from a 2^n factorial in terms of (0,1)-matrices.

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The question now arises as to whether or not a similar transformation of X to an X^* can be found for the $\prod_{i=1}^n s_i$ factorial. This is accomplished in section 2 of the paper and an X^* is found which is a $(0,1)$ -matrix. Thus the determinant of $X'X$ and of $X^{*'}X^*$ can be represented in terms of $(0,1)$ -matrices. This offers a new approach to the construction of generalized main effect plans for both symmetrical and asymmetrical factorials. Two theorems of Raktoc and Federer [1970] for the 2^n factorial are extended to include the s^n factorial (theorems 2.1 and 2.2) and the $\prod_{i=1}^n s_i$ factorial (theorems 2.3 and 2.4).

In the third section we obtain an upper bound on the determinant of X^* , or X , for saturated main effect plans from the s^n factorial (theorem 3.1) and from the $\prod_{i=1}^n s_i$ factorial (theorem 3.2). A lower bound for the determinant of X^* for nonsingular main effect plans is obtained in theorem 3.3. Three methods of constructing saturated main effect plans are described in section 4. Using these results, some possible values of the determinants of X^* , and of X , are presented in theorem 4.1. The fifth section of the paper is concerned with five methods of constructing both saturated and unsaturated main effect plans for both symmetrical and asymmetrical factorials.

If D is an orthogonal main effect plan derived from a set of orthogonal latin squares, the maximum possible value for determinant of $X^{*'}X^*$ is given in theorem 5.1; the corresponding value for a design obtained from an orthogonal array is given in theorem 5.2.

The usefulness of representing the design matrix D in terms of $(0,1)$ -matrices and of transforming X to X^* is illustrated with examples throughout the paper. This new approach offers solutions to some of the problems associated with main effect plans and their variance optimality property.

2. Representation of Factorial Main Effect Plans in Terms of (0,1)-matrices. First let us consider the s^n symmetrical factorial and the corresponding main effect plan for estimating the $v = 1 + n(s-1)$ mean and main effects under the assumption that all two-factor and higher-factor interactions are zero. Let $T(N \times n)$ be an $N \times n$ matrix, $N \geq v$, with elements from the set $\{0, 1, \dots, s-1\}$ denoting such a main effect plan. Let T_i , $i = 0, 1, \dots, s-1$, be the $N \times n$ incidence matrix of element i in T . That is, an element of T_i is one or zero as the corresponding element of T is i or not. Then,

$$\sum_{i=0}^{s-1} T_i = J_{Nn}, \quad (2.1)$$

and

$$T = \sum_{i=0}^{s-1} iT_i.$$

Typically main effects are defined in terms of a set of orthogonal polynomials. For convenience, we shall use the Helmert polynomials,

$$\begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & -1 & 0 & & 0 \\ 1 & 1 & -2 & & 0 \\ \vdots & & & \ddots & \\ 1 & 1 & 1 & \dots & -(s-1) \end{bmatrix}, \quad (2.3)$$

even though any set may be used. Then, if \underline{y} denotes an $N \times 1$ observation vector corresponding to T , we shall consider the following relations for \underline{y} to hold:

$$E[\underline{y}] = X\beta \text{ and } \text{Cov}(\underline{y}) = \sigma^2 I_n, \quad (2.4)$$

where $\beta' = (\mu, B_1, \dots, B_n, B_1^2, \dots, B_n^2, B_1^3, \dots, B_n^{s-1}, \dots, B_n^{s-1})$ denotes the $v \times 1$ parameter vector of single degree of freedom contrasts as derived from Helmert polynomials and where X is the design matrix. The design matrix may be written as

$$X = \begin{bmatrix} 1 & : & T_0 - T_1 & : & T_0 + T_1 - 2T_2 & : & \dots & : & \sum_{i=1}^{s-2} T_i - (s-1)T_{s-1} \end{bmatrix}. \quad (2.5)$$

We shall next show how to transform a design matrix X for a main effect plan from the s^n factorial into a $(0,1)$ -matrix. Thus, a characterization of main effect plans will be made in terms of $(0,1)$ -matrices and a means is provided whereby the optimality of such plans may be studied. The results obtained are embodied in theorems 2.1 and 2.2 for the s^n factorial and in theorems 2.3 and 2.4 for the general $\prod_{i=1}^k s_i^{n_i}$ asymmetrical factorial. The importance of these results centers around the facts that (i) considerable theory is available on the construction of main effect plans for the 2^n factorial and on the values of the determinants of $(0,1)$ -matrices (see, for example, Anderson and Federer [1974]), (ii) this theory can now be applied to the construction and to the consideration of optimality of main effect plans from the general factorial, and (iii) these results extend the results of Raktoe and Federer [1970] for the 2^n factorial to the general symmetrical and asymmetrical factorials.

Now, consider the column operations on X resulting from postmultiplying by a matrix G as follows:

$$XG = X^*, \quad (2.6)$$

where G is the following $v \times v$ matrix:

$$G = \begin{bmatrix} 1 & \frac{1'}{s} & \frac{1'}{s} & \frac{1'}{s} & \dots & \frac{1'}{s} & \frac{1'}{s} \\ 0 & -I_n/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & I_n/2(3) & -I_n/3 & 0 & 0 & 0 & 0 \\ 0 & I_n/3(4) & I_n/3(4) & -I_n/4 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & I_n/(s-2)(s-1) & I_n/(s-2)(s-1) & I_n/(s-2)(s-1) & \dots & -I_n/(s-1) & 0 \\ 0 & I_n/s(s-1) & I_n/s(s-1) & I_n/s(s-1) & \dots & I_n/s(s-1) & -I_n/s \end{bmatrix}. \quad (2.7)$$

Theorem 2.1. Under the transformation G, we have

(a) $X^* = [\frac{1}{s} : T_1 : T_2 : \dots : T_{s-1}]$, that is, the transformed design matrix is a (0,1)-matrix composed of incidence matrices T_i , $i=1,2,\dots,s-1$;

(b) $|G| = (s!)^{-n}(-1)^{n(s-1)} ;$

(c)

$$G^{-1} = \begin{bmatrix} 1 & \frac{1'}{s} & \frac{1'}{s} & \frac{1'}{s} & \dots & \frac{1'}{s} & \frac{1'}{s} \\ 0 & -2I_n & 0 & 0 & 0 & 0 & 0 \\ 0 & -I_n & -3I_n & 0 & 0 & 0 & 0 \\ 0 & -I_n & -I_n & -4I_n & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & -I_n & -I_n & -I_n & \dots & -(s-1)I_n & 0 \\ 0 & -I_n & -I_n & -I_n & \dots & -I_n & -sI_n \end{bmatrix};$$

(d) $X = X^*G^{-1} ;$ and

(e) $|X'X| = (s!)^{2n}|X^{*'}X^*| .$

Theorem 2.2. If $N = v$, and thus the design is a saturated main effect plan, the determinant of the resulting square matrix may be expressed as:

$$|X| = (-1)^{n(s-1)}(s!)^n|X^*| .$$

The proof follows directly from parts (a), (b), and (d) of theorem 2.1.

Example 2.1. To illustrate the results of theorems 2.1 and 2.2, consider the saturated main effect plan for the 3^4 factorial derived from the following pair of orthogonal latin squares:

$$L_1(3) = \begin{bmatrix} 0 & 1 & 2 \\ 1 & 2 & 0 \\ 2 & 0 & 1 \end{bmatrix} \quad \text{and} \quad L_2(3) = \begin{bmatrix} 0 & 1 & 2 \\ 2 & 0 & 1 \\ 1 & 2 & 0 \end{bmatrix}$$

Then,

$$T = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 2 & 2 & 2 \\ 1 & 0 & 1 & 2 \\ 1 & 1 & 2 & 0 \\ 1 & 2 & 0 & 1 \\ 2 & 0 & 2 & 1 \\ 2 & 1 & 0 & 2 \\ 2 & 2 & 1 & 0 \end{bmatrix}, \quad T_1 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad \text{and} \quad T_2 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \end{bmatrix}.$$

The determinant of X is $|X| = (3!)^4 \begin{bmatrix} 1 \\ T_1 \\ T_2 \end{bmatrix} = (3!)^4(27)$, and since T is an orthogonal array, this is the maximum value possible (see next section).

The effect of the structure constraints (2.1) and (2.2) on T_0 , T_1 , and T_2 is apparent from example 2.1. The value 27 is far below the maximum value of the determinant of a 9×9 (0,1)-matrix with a leading column of ones. In fact, for such matrices, Anderson and Federer [1974] obtained the following values: all integers $\leq 33, 36, 40, 44, 48$, and 56, with no assurance that all values of the determinant of (9×9) (0,1)-matrices have been obtained or that 56 is the maximum value. Thus, the largest value for (9×9) (0,1)-matrices subject to constraints (2.1) and (2.2) is an intermediate value among the possible values of the determinants.

We now generalize the results for the s^n factorial to the general asymmetrical factorial $s_1^{n_1} \times s_2^{n_2} \times \dots \times s_k^{n_k} = \prod_{i=1}^k s_i^{n_i}$. For n_i factors at levels s_i for each value of i , denote the matrix G of (2.7) as

$$G_i = \begin{bmatrix} 1 & \underline{1}'/s_i \\ 0 & H_i \end{bmatrix},$$

and the corresponding matrix X^* as $X_i^* = [\underline{1} \ Z_i^*]$. Then, for the asymmetrical case,

$$G = \begin{bmatrix} 1 & \underline{1}'/s_1 & \underline{1}'/s_2 & \dots & \underline{1}'/s_k \\ 0 & H_1 & 0 & & 0 \\ 0 & 0 & H_2 & & 0 \\ \vdots & & & & \vdots \\ 0 & 0 & 0 & \dots & H_k \end{bmatrix}. \quad (2.8)$$

It can be ascertained that if X is the design matrix for a main effect plan from the asymmetrical factorial that the following two theorems hold:

Theorem 2.3. (a) $XG = X^* = [\underline{1} : Z_1^* : Z_2^* : \dots : Z_k^*]$, where X^* is a $(0,1)$ -matrix with leading column $\underline{1}$;

(b) $|G| = \prod_{i=1}^k (s_i!)^{-n_i}$; and

(c) $|X'X| = \prod_{i=1}^k (s_i!)^{2n_i} |X^{*'}X^*|$

Theorem 2.4. If T is a saturated main effect plan for the asymmetrical $\prod_{i=1}^k s_i^{n_i}$ factorial, then

$$|X| = \prod_{i=1}^k (s_i!)^{n_i} |\underline{1} : Z_1^* : Z_2^* : \dots : Z_k^*|.$$









3. An Upper Bound and a Lower Bound on the Value of the Determinant of Nonsingular Design Matrices. The value (absolute values only are considered) of the determinant of the X matrix for a saturated main effect plan from the generalized symmetrical or asymmetrical factorial, is invariant under any change of level designation for any specified factor. This has been proved by Paik and Federer [1970] and by Srivastava, Raktoe, and Pesotan [1971]. However

under the transformation from X to X^* , this fact can be easily demonstrated. A relabeling of any nonzero level for any given factor results in an interchange in columns of X^* , which does not alter the value of the determinant. Likewise, any nonzero level may be interchanged with the zero level for any specified factor by taking the appropriate linear combination of the first column of X^* and the columns of X^* for the particular factor involved; here again the value of the determinant of X^* remains unchanged. Likewise, the value of the determinant of X^* remains invariant under a permutation of factors having the same levels (Joiner [1973]). Hence the transformation from X to X^* is important in providing a simple proof for an invariance result, and we shall see other uses throughout this paper. In theorems 3.1 and 3.2, we have been able to place an upper bound on the determinant of X^* , and consequently X . Also, in theorem 3.3 we have obtained the lowest possible value for matrices X^* and X . These results were made possible using the transformation from X to X^* .

Let δ_i^k , $k = 0, 1, 2, \dots, s-1$ denote the number of combinations of a fraction T which contain the i^{th} factor at level k . Then, $\sum_{k=0}^{s-1} \delta_i^k$ for each i . In any discussion involving the determinant of X , or of X^* , we may, without loss of generality, assume that $\delta_i^0 \geq \delta_i^1 \geq \delta_i^2 \geq \dots \geq \delta_i^{s-1}$ for each i because of the invariance property discussed above.

Raktoe and Federer [1970] obtained the following bound on $\|X^*\|$ using Hadamard's theorem:

$$\|X^*\| \geq (n+1)^{(n+1)/2} 2^{-n} \quad (3.1)$$

Since $\|X^*\|$ must be an integer, we take the integer part of the right hand side of (3.1) as the upper bound. We now obtain a generalization of their result for X^* matrices, and consequently X matrices, for saturated main effect plans from the symmetrical s^n factorial.

Theorem 3.1. Let T be a saturated main effect plan for the s^n factorial with $N = n(s-1) + 1$. If $X^* = [1 : T_1 : T_2 : \dots : T_{s-1}]$, then

$$|X^*| \leq \text{integer part of } N^{N/2} s^{-sn/2}. \quad (3.2)$$

When $s = 2$, this reduces to Hadamard's bound.

Proof: From theorem 2.2,

$$\|X^*\| = (s!)^{-n} \|X\| = (s!)^{-n} |X'X|^{1/2}. \quad (3.3)$$

From Hadamard's determinant theorem, we know that $|X'X|$ is less than or equal to the product of its diagonal elements with equality only if $X'X$ is a diagonal matrix. Using equations (2.5) and (3.3), we obtain:

$$\|X^*\| \leq (s!)^{-n} N \prod_{i=1}^n \prod_{k=1}^{s-1} (\delta_i^0 + \delta_i^1 + \dots + \delta_i^{k-1} + k^2 \delta_i^k), \quad (3.4)$$

where we take $\delta_i^0 \geq \delta_i^1 \geq \dots \geq \delta_i^{s-1}$ for each i .

Expression (3.4) will be maximized whenever each of the interior products is maximized; thus, we need only consider

$$\prod_{k=1}^{s-1} (\delta_i^0 + \delta_i^1 + \dots + \delta_i^{k-1} + k^2 \delta_i^k). \quad (3.5)$$

Now, introduce the Lagrange multiplier corresponding to the constraint $\sum_{k=1}^{s-1} \delta_i^k - N = 0$, and then take derivatives with respect to δ_i^{s-2} and δ_i^{s-1} . Equating these two derivatives, we obtain an expression in δ_i^{s-2} and δ_i^{s-1} as follows:

$$\delta_i^{s-2} = \frac{(s-2)^2 + 1}{(s-1)(s-3)} \delta_i^{s-1} - \frac{2N}{s(s-1)(s-3)}. \quad (3.6)$$

The equations are satisfied when $\delta_i^{s-2} = \delta_i^{s-1} = N/s$. We may assume that $\delta_i^{s-2} \geq \delta_i^{s-1}$ and that $\delta_i^{s-1} \leq N/s$ from the ordering previously described.

Whenever $\delta_i^{s-1} < N/s$, we have $\delta_i^{s-2} < \delta_i^{s-1}$ from (3.6). Hence, it follows that $\delta_i^{s-1} = \delta_i^{s-2} = N/s$ and since the smallest of the δ_i^k equals N/s and since their total is N , we have

$$\delta_i^0 = \delta_i^1 = \delta_i^2 = \dots = \delta_i^{s-1} = N/s, i = 1, 2, \dots, n. \quad (3.7)$$

Thus,

$$\begin{aligned} \|X^*\| &\leq (s!)^{-n} \left\{ N^N \left(\frac{s-1}{\prod_{k=1}^{s-1} k(k+1)} \right)^n s^{-N+1} \right\}^{1/2} \\ &= (s!)^{-n} N^{N/2} [(s-1)!s!]^{n/2} s^{-n(s-1)/2} \\ &= N^{N/2} s^{-ns/2}, \end{aligned}$$

which completes the proof.

The upper bound for the general asymmetrical factorial may be proved in a similar manner since the maximization is essentially for a single factor at a time. The results are embodied in the following theorem:

Theorem 3.2. Let T be a saturated main effect plan for the general asymmetrical $\prod_{i=1}^k s_i^{n_i}$ factorial with $N = 1 + \sum_{i=1}^k n_i(s_i - 1)$ runs and let X^* be the $(0,1)$ -matrix of theorems 2.3(a) and 2.4. Then,

$$|X^*| \leq \text{integer part of } N^{N/2} \prod_{i=1}^k s_i^{-s_i n_i / 2}.$$

Example 3.1. To illustrate the usefulness of theorems 3.1 and 3.2, consider the class of 8×8 $(0,1)$ -matrices with a leading column of ones. The Hadamard bound for this case is 32 and is attainable. The possible values of the determinants in this class are: all integers ≤ 18 , 20, 24, and 32, with all other integer values < 32 being unattainable. Let (k_1, k_2, \dots, k_r) denote an $N \times N$ $(0,1)$ -matrix with a set of k_1 mutually disjoint columns, a second set of k_2 mutually disjoint columns, ..., and an r^{th} set of k_r mutually disjoint columns.

Such a $(0,1)$ -matrix could be considered as an X^* for a $(k_1+1) \times (k_2+1) \times \dots \times (k_r+1)$ saturated main effect plan. Using theorem 3.2, table 1 has been constructed and gives the bounds on various partitions for $N = 8$. For example, the second number in the table is obtained as the integer part of $8^4(3^{-3/2})(2^{-5})$ which is 24.

We now turn our attention to the lowest possible value attainable for the matrices X and X^* and show how to construct such plans. The one-at-a-time procedure of holding the levels of all factors but one fixed and then running through all levels of the factor not fixed produces plans similar to the following:

$$\begin{array}{cccc} 0 & 0 & \dots & 0 \\ 1 & 0 & & 0 \\ \vdots & & & \\ s_1-1 & 0 & & 0 \\ 0 & 1 & & 0 \\ \vdots & & & \\ 0 & s_2-1 & & 0 \\ \vdots & & & \\ 0 & 0 & & 1 \\ \vdots & & & \\ 0 & 0 & \dots & s_n-1 \end{array}$$

Plans derived by this procedure produce the "least optimal" plans in the sense that the minimum nonzero determinant value of X is attained by these plans. The characterization of section 2 provides a simple proof that these designs are least optimal. The results are contained in the following theorem:

Theorem 3.3. For saturated main effect plans from the $\prod_{i=1}^k s_i^{n_i}$ factorial, the minimum possible nonzero value of $X'X$ is attained by the one-at-a-time design. The minimal value on $|X'X|$ is

Table 1. Upper bounds on $|X^*|$ with $N = 8$.

<u>Column Structure</u>	<u>Representation</u>	<u>Bound</u>
(1,1,1,1,1,1,1)	2^7	32
(2,1,1,1,1,1)	3×2^5	24
(3,1,1,1,1)	4×2^4	16
(4,1,1,1)	5×2^3	9
(5,1,1)	6×2^2	4
(6,1)	7×2	2
(7)	8	1
(2,2,1,1,1)	$3^2 \times 2^3$	18
(2,2,2,1)	$3^3 \times 2$	14
(3,2,1,1)	$4 \times 3 \times 2^2$	12
(3,2,2)	4×3^2	9
(3,3,1)	$4^2 \times 2$	8
(4,2,1)	$5 \times 3 \times 2$	7
(4,3)	5×4	4
(5,2)	6×3	3

$$|X'X| = |G^{-1}|^2 |X^*X^*| = |G^{-1}|^2 = \prod_{i=1}^k (s_i!)^{2n_i}.$$

Proof: For this design it can be shown that

$$X^* = \begin{bmatrix} 1 & 0'_{1 \times (N-1)} \\ \vdots & \vdots \\ 1_{(N-1) \times 1} & I_{(N-1)} \end{bmatrix},$$

for $N = 1 + \sum_{i=1}^k n_i(s_i - 1)$, and that $\|X^*\| = 1$, the minimum nonzero integer.

Thus the smallest nonzero value of the determinant of X , or X^* , can always be attained. The upper bound on the determinant of X , or X^* , will be attained whenever an orthogonal saturated main effect plan with equal numbers of repetitions on the levels of each factor is obtained. In the 3^n series, for example, this will occur with $n = 4$ and $N = 9$ yielding $|X^*| = 3^3$; the next orthogonal saturated main effect plan occurs for $n = 13$, and $N = 27$ yielding $|X^*| = 3^{21}$. In cases where an orthogonal plan does not exist the upper bound will not be achieved.

4. Three Methods of Constructing Saturated Main Effect Plans and Some Possible Values of the Determinant of X . A method of constructing saturated main effect plans was given in the previous section and was called the one-at-a-time procedure. These designs belong to the class of least variance-optimal designs, and hence any other method of construction should result in more variance-optimal designs. The construction of a saturated main effect plan for the asymmetrical factorial is a problem of constructing a $(0,1)$ -matrix under constraints (2.1) and (2.2). The first method described is (i) to obtain an $N \times N$ $(0,1)$ -matrix with a large determinant, (ii) to choose sets of columns to conform with the necessary column structure, and (iii) to change systematically ones to zeros in order to attain disjoint columns. It may be necessary

to change additional ones in one or more columns in order that the δ_i^k 's are as nearly equal to N/s_i as possible.

Example 4.1. The following (0,1)-matrix is obtained from a Hadamard matrix of order 8, by changing minus ones to zeros; it has a determinant of 32.

1	1	1	1	1	1	1	1
1	0	1	0	1	0	1	0
1	1	0	0	1	1	0	0
1	0	0	1	1	0	0	1
1	1	1	1	0	0	0	0
1	0	1	0	0	1	0	1
1	1	0	0	0	0	1	1
1	0	0	1	0	1	1	0

As illustrated in table 2, we may obtain a series of saturated main effect plans by changing various ones to zeros. For example, a change of the row-column coordinates indicated produces the first plan:

$$X^* = \begin{bmatrix} 1 & \boxed{0} & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & \boxed{0} & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \end{bmatrix} \text{ and } T = \begin{bmatrix} 2 & 1 & 1 & 1 & 1 & 1 \\ 2 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 \end{bmatrix}$$

The second method presented represents a more direct approach to the construction of the desired matrix for the 3^n series. The method may be easily extended for the s^n factorial. A matrix of the form

$$C_{m+1} = \begin{bmatrix} c_0 & c_1 & c_2 & \cdots & c_m \\ c_m & c_0 & c_1 & & c_{m-1} \\ c_{m-1} & c_m & c_0 & & c_{m-2} \\ \vdots & & & & \vdots \\ c_1 & c_2 & c_3 & \cdots & c_0 \end{bmatrix}$$

Table 2.

<u>Factorial Type</u>	<u>Change Coordinates</u>	<u>Determinant</u>
3×2^5	(1,2), (5,3)	12
$3^2 \times 2^3$	(1,k), k=2, 3, ..., 8 (5,3), (4,5)	10
$3^3 \times 2$	(1,k), k=2, 3, ..., 8 (5,3), (4,5), (8,7)	6
4×2^4	(1,2), (1,3), (1,4) (5,2), (5,3), (5,4)	16
$4 \times 3 \times 2^2$	(1,2), (1,3), (1,4) (5,2), (5,3), (5,4) (1,5), (3,6)	8

is called a circulant. Construct X^* as follows:

$$X^* = \begin{bmatrix} 1 & 0'_{1 \times (N-1)} \\ 1_{(N-1) \times 1} & C_{N-1} \end{bmatrix}$$

where c_i , $i=0, 1, \dots, N-2$ are either zero or one, and where $N = 1 + 2n$. Partition C into 2 sets of n columns each, $C = [C_1 : C_2]$ where C_1 consists of the first n columns and C_2 the last n columns. The i^{th} and $(n+i)^{\text{th}}$ columns of X^* are disjoint if c_i and c_{n+i} are not both one, $i=0, 1, \dots, n-1$. Thus, we have a necessary and sufficient condition on C which results in an X^* matrix with the desired column structure for the 3^n factorial. We list here the first row of a suitable C matrix for $n = 3, 4, 5, 6$, and, 7 for the 3^n factorial with the corresponding value of the determinant:

<u>n</u>	<u>First Row of C</u>	<u>Determinant of X^*</u>
3	(1 0 1 0 0 0)	4
4	(1 1 0 1 0 0 0 0)	27
5	(1 1 1 0 1 0 ... 0)	88
6	(1 1 1 0 1 0 ... 0)	208
7	(1 1 0 1 1 0 1 0 ... 0)	420

For the third method of constructing a saturated main effect plan for the s^n factorial, let the $n \times n$ (0,1)-matrices be of the form:

$$\begin{bmatrix} 0' \\ - \\ T_i \end{bmatrix} \quad i = 1, 2, \dots, s-1$$

Each of these could be regarded as a saturated main effect plan for the 2^n factorial. Now let the design T be

$$T = \begin{bmatrix} 0' \\ T_1 \\ 2T_2 \\ \vdots \\ (s-1)T_{s-1} \end{bmatrix} .$$

For this design,

$$X^* = \begin{bmatrix} 1 & 0' & 0' & \dots & 0' \\ 1 & T_1 & 0 & & 0 \\ 1 & 0 & T_2 & & 0 \\ \vdots & & & & \vdots \\ 1 & 0 & 0 & \dots & T_{s-1} \end{bmatrix} ,$$

and $|X^*| = \prod_{i=1}^{s-1} |T_i|$. From these results, we now state theorem 4.1:

Theorem 4.1. Some possible values for the determinant of X for saturated main effect plans from the s^n factorial, are

$$|X| = (s!)^n \prod_{i=1}^{s-1} |T_i| ,$$

where the T_i , $i=1, 2, \dots, s-1$, are $n \times n$ (0,1)-matrices.

Anderson and Federer [1974] considered possible values for the determinant of (0,1)-matrices and used ten methods of construction to obtain many of the possible values. In the following example, we present all possible determinant values attainable by the above method of construction for saturated main effect plans from the 3^n series for $n=3, 4, 5, 6$, and 7.

Example 4.1. From theorem 4.1, we note that the following values for $n=3, 4, 5, 6$, and 7 for the 3^n series are attainable:

$$n = 3: 6^3[0,1,2,4]$$

$$n = 4: 6^4[0,1,2,3,6,9]$$

$$n = 5: 6^5[0,1,2,3,4,5,6,8,9,10,12,15,20,25] = 6^5\left[[0,1,2,3,4,5]^2\right]$$

$$n = 6: 6^6[0,1,2,\dots,9]^2 = 6^6[\text{all possible products of integers } 0,1,\dots,9]$$

$$n = 7: 6^7[\text{all integers } \leq 18,20,24,32]^2$$

where the integers within a square bracket represent possible values for the determinant of X^* .

It should be noted that this construction is restrictive and does not provide all possible values of $|X|$. For example, for $n = 3$, and for another construction, it is possible to obtain a design for which $|X| = 6^3(3)$ and which is not obtained via the above construction. Even though the third method of construction gave the largest value obtained for $n = 3$, it is not expected that this will hold for larger n . When $n = 4$, the orthogonal saturated design in example 2.1 yields a design for which $|X| = 6^4(27)$, which is three times larger than the largest value obtained from theorem 4.1. The spectrum of possible values or even the largest possible value of $|X|$ is unknown at present. The transformation of X to X^* , i.e., a $(0,1)$ -matrix, is considered to be one step toward the resolution of these problems.

5. Main Effect Plans in General. The representation of the design matrix X in terms of the $(0,1)$ -incidence matrix X^* provides a new avenue of approach in the construction of symmetrical and asymmetrical main effect plans, both saturated and unsaturated. In this section, we discuss X^* matrices as obtained from four methods: theorem 4.1, orthogonal latin squares, orthogonal arrays, and the collapsing of levels in an orthogonal main effect plan. An additional construction is presented for the s^n series, which uses a design T and its complement $(J-T)$. An obvious necessary condition for nonsingularity of a main

of a main effect plan T is that each T_i , $i=0, 1, \dots, s-1$, be nonsingular. Furthermore, there can be no linear dependencies among the columns of the T_i . The initial constraint (2.1) states that for each position there must be exactly one one with the rest being zeros in the incidence matrices T_i , $i=0, 1, 2, \dots, s-1$.

The construction of theorem 4.1 can be extended to the general main effect plans. Let T_1, T_2, \dots, T_{s-1} be $(0,1)$ -matrices of order $N_1 \times n, N_2 \times n, \dots, N_{s-1} \times n$, respectively, for $N_i \geq n$, such that $[0 \ T_1']'$ could be regarded as a main effect plan for the 2^n factorial with $N_1 + 1$ runs. Now, consider the following design for the s^n factorial with $N = 1 + \sum_{i=1}^{s-1} N_i$ runs:

$$[0 \ T_1' \ 2T_2' \ \dots \ (s-1)T_{s-1}']'$$

Then,

$$X^* = \begin{bmatrix} 1 & 0' & 0' & \dots & 0' \\ 1 & T_1 & 0 & & 0 \\ 1 & 0 & T_2 & & 0 \\ \vdots & & & & \vdots \\ 1 & 0 & 0 & \dots & T_{s-1} \end{bmatrix},$$

and

$$X^{*'}X^* = \begin{bmatrix} N & 1'T_1 & 1'T_2 & \dots & 1'T_{s-1} \\ T_1'1 & T_1'T_1 & 0 & & 0 \\ T_2'1 & 0 & T_2'T_2 & & 0 \\ \vdots & & & & \vdots \\ T_{s-1}'1 & 0 & 0 & \dots & T_{s-1}'T_{s-1} \end{bmatrix}.$$

Given the T_i , $i=1, 2, \dots, s-1$, it is a relatively simple matter to compute $|X^{*'}X^*|$.

Next consider a set of t orthogonal latin squares of order s . This set may be regarded as an orthogonal main effect plan for the s^{t+2} factorial with $N = s^2$. If $t = s-1$, which exists whenever s is a prime or prime power, the set forms an orthogonal saturated main effect plan. The $s^2 \times (1 + (t+2)(s-1))$ matrix X^* is given by

$$X^* = \begin{bmatrix} \underline{1} & T_1 & T_2 & \cdots & T_{s-1} \end{bmatrix}$$

and since $T_i' T_i = (s-1)I + J$ and $T_i' T_j = J - I$, $i \neq j$, we have

$$X^{*'} X^* = \begin{bmatrix} s^2 & s\underline{1}' & s\underline{1}' & \cdots & s\underline{1}' \\ s\underline{1} & sI+(J-I) & J-I & & J-I \\ s\underline{1} & J-I & sI+(J-I) & & J-I \\ \vdots & & & \ddots & \\ s\underline{1} & J-I & J-I & \cdots & sI+(J-I) \end{bmatrix}$$

The determinant of $X^{*'} X^*$ is $|X^{*'} X^*| = s^{(t+2)(s-2)+2}$. When $t = s-1$ and we have a saturated main effect plan,

$$|X^{*'} X^*| = s^{s(s-1)}$$

and

$$|X^*| = s^{s(s-1)/2}.$$

These values represent maximum values of the determinant of $X^{*'} X^*$, and by theorem 2.1, the corresponding values of $|X'X|$. More important is the fact that for the s^n factorial and for $i = j = 1, 2, \dots, s-1$,

$$T_i' T_i = sI + (J-I) \text{ and } T_i' T_j = J - I,$$

which is a characteristic of orthogonal designs and which provides some insight into the structure of optimal designs for other values of N . This information is summarized in the following theorem:

Theorem 5.1. If T is an orthogonal main effect plan for the s^{t+2} factorial and is obtained from a set of t orthogonal latin squares, then in the representation of theorem 2.1,

$$T_1' T_1 = sI + (J-I) \text{ and } T_1' T_j = J - I, \quad i \neq j = 1, 2, \dots, s-1.$$

The maximum possible value for $|X^* X^*|$ with s^2 observations is $|X^* X^*| = s^{(t+2)(s-2)+2}$. If $t = s-1$, $|X^*| = s^{s(s-1)/2}$.

A similar structure is obtained for a general orthogonal array with N runs, n factors, in s symbols, of strength 2, and denoted by $(N, n, s, 2)$. Let λ_2 denote the number of runs which contain any pair of levels of any pair of factors and let $r = N/s$. Then,

$$X^* X^* = \begin{bmatrix} N & r\mathbf{1}' & r\mathbf{1}' & \dots & r\mathbf{1}' \\ r\mathbf{1} & rI_n + \lambda_2(J-I_n) & \lambda_2(J-I_n) & & \lambda_2(J-I_n) \\ r\mathbf{1} & \lambda_2(J-I_n) & rI_n + \lambda_2(J-I_n) & & \lambda_2(J-I_n) \\ \vdots & & & \ddots & \\ r\mathbf{1} & \lambda_2(J-I_n) & \lambda_2(J-I_n) & \dots & rI_n + \lambda_2(J-I_n) \end{bmatrix},$$

and

$$|X^* X^*| = r^{n(s-2)} [r - \lambda_2(n-1)] [rN + N\lambda_2(n-1)(s-1) - n(s-1)r^2].$$

Theorem 5.2. If T is an $(N, n, s, 2)$ orthogonal array, then in the representation of theorem 2.1,

$$T_1' T_1 = rI_n + \lambda_2(J-I) \text{ and } T_1' T_j = \lambda_2(J-I_n), \quad i \neq j = 1, 2, \dots, s-1,$$

and

$$|X^* X^*| = r^{n(s-2)} [r - \lambda_2(n-1)] [rN + N\lambda_2(n-1)(s-1) - n(s-1)r^2].$$

A set of t orthogonal latin squares of order s forms a $(s^2, t, s, 2)$ orthogonal array with $\lambda_2 = 1$. The existence of a group divisible partially

balanced incomplete block design with parameters $v = ns$, $b = \lambda_2 n^2$, $k = n$, $r = s\lambda_2$, $\lambda_1 = 0$, and λ_2 is equivalent to the existence of a $(\lambda_2 n^2, n, s, 2)$ orthogonal array. There is a convenient table given by Clatworthy [1973], for obtaining a large number of such arrays with $r \leq 10$. Also, a set of t orthogonal $F(n, \lambda)$ F-squares has been given by Hedayat and Seiden [1970] and may be used to form a $(n^2, t+2, n/\lambda, 2)$ orthogonal array with $r = n\lambda$ and $\lambda_2 = \lambda^2$.

The next method of construction considered is that of collapsing levels in an orthogonal main effect plan from the s^n factorial. For example, a 3^6 main effect plan in 25 runs might be constructed from the set of four orthogonal latin squares of order 5 by the mapping

$$\begin{array}{rcl} 0 & \rightarrow & 0 \\ 1 & \rightarrow & 1 \\ 2 & \rightarrow & 1 \\ 3 & \rightarrow & 2 \\ 4 & \rightarrow & 2 \end{array}$$

that is, levels 1 and 2 collapse to level 1 and levels 3 and 4 collapse to level 2. This design would permit estimation of the 13 mean and main effect parameters in the absence of interactions and would allow 12 degrees of freedom to estimate the error variance. In X^* , the collapsing of levels is equivalent to adding incidence matrices. If U_0 , U_1 , and U_2 denote the incidence matrices of 0's, 1's, and 2's in the above example, then

$$\begin{array}{l} U_0 = T_0 \\ U_1 = T_1 + T_2 \\ U_2 = T_3 + T_4, \end{array}$$

where the T_i , $i = 0, 1, 2, 3, 4$, are the incidence matrices for the design before collapsing.

In general suppose that we have an orthogonal main effect plan for the s^n factorial and that we make the following mapping of levels:

$$i_1 \rightarrow i, i_2 \rightarrow i, \dots, i_k \rightarrow i$$

and

$$j_1 \rightarrow j, j_2 \rightarrow j, \dots, j_m \rightarrow j$$

Then,

$$U_i = \sum_{h=1}^k T_{ih} \text{ and } U_j = \sum_{h=1}^m T_{jh}$$

It follows that

$$U_i' U_i = krI_n + k^2 \lambda_2 (J-I)$$

and

$$U_i' U_j = km \lambda_2 (J-I)$$

Thus, $X^* X^*$ is expressible directly in terms of the above matrices in the same form as given for latin squares and orthogonal array X^* 's.

Suppose that an asymmetrical main effect plan is obtained by collapsing levels of an orthogonal main effect plan. For example, a $2^2 \times 3^2 \times 4 \times 5$ main effect plan may be obtained from the four orthogonal latin squares of order five by the mapping:

	Factors			
	<u>1 & 2</u>	<u>3 & 4</u>	<u>5</u>	<u>6</u>
0 →	0	0	0	0
1 →	0	1	1	1
2 →	1	1	2	2
3 →	1	2	3	3
4 →	1	2	3	4

The design permits estimation of the 14 mean and main effect parameters in the absence of interactions and permits estimation of an error variance with 11 degrees of freedom. The operation of collapsing levels again corresponds to adding corresponding columns of the incidence matrices T_i .

Each of the above two examples is a special case of orthogonal F-squares. The method of collapsing levels is only one of several methods for constructing orthogonal F-squares. This method is not available when orthogonal latin squares do not exist, as for example with 6×6 squares.

To conclude, we suggest one additional construction for main effect plans from the s^n factorial. This method makes use of a $(0,1)$ -matrix T and its complement $(J-T)$ and by arranging these matrices to satisfy constraints (2.1) and (2.2). We illustrate the procedure for the 3^n , the 4^n series, and then for the s^n series.

Let T be an $N \times n$ $(0,1)$ -matrix of full rank with $N \geq n$. For the 3^n series, consider the plan defined by

$$T_1 = \begin{bmatrix} T \\ J - T \\ 0 \end{bmatrix} \quad \text{and} \quad T_2 = \begin{bmatrix} 0 \\ T \\ J - T \end{bmatrix}$$

with $3N$ runs. Each of the three levels of each factor occurs N times. For this design,

$$X^*X^* = \begin{bmatrix} 3N & N\underline{1}' & N\underline{1}' \\ N\underline{1} & T'T + (J-I)'(J-T) & (J-T)'T \\ N\underline{1} & T'(J-T) & T'T + (J-T)'(J-T) \end{bmatrix}.$$

If T itself is an orthogonal array, then X^*X^* has a simple structure. For example, if $T = I_n$, then

$$X^*X^* = \begin{bmatrix} 3n & n\underline{1}' & n\underline{1}' \\ n\underline{1} & nI + (n-2)(J-I) & (J-I) \\ n\underline{1} & (J-I) & nI + (n-2)(J-I) \end{bmatrix}$$

and

$$|X^*X^*| = 3^{n-1}n(n^2-3n+3)^2.$$

For the 4^n series, the construction is given by

$$T_1 = \begin{bmatrix} T \\ J - T \\ 0 \\ 0 \end{bmatrix}, T_2 = \begin{bmatrix} 0 \\ T \\ J - T \\ 0 \end{bmatrix}, \text{ and } T_3 = \begin{bmatrix} 0 \\ 0 \\ T \\ J - T \end{bmatrix}$$

In general, for the s^n factorial we let T_i , $i = 1, 2, \dots, s-1$, be $sN \times n$ matrices whose i^{th} and $(i+1)^{\text{st}}$ blocks are T and $J - T$, respectively, with the remaining blocks composed of zero matrices. For this construction, we have:

$$X^*X^* = \begin{bmatrix} sN & N_1' & N_1' & N_1' & \dots & N_1' \\ N_1 & A & B & 0 & & 0 \\ N_1 & B & A & B & & 0 \\ N_1 & 0 & B & A & & 0 \\ \vdots & & & & & \vdots \\ N_1 & 0 & 0 & 0 & \dots & A \end{bmatrix},$$

where $A = T'T + (J-T)'(J-T)$ and $B = (J-T)'T$.

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References

- [1] Anderson, D. A. and W. T. Federer (1974). Possible absolute determinant values for square $(0,1)$ -matrices useful in fractional replication. No. BU-493-M in the Mimeo Series of the Biometrics Unit, Cornell University, January.
- [2] Clatworthy, W. H. (1973). Tables of two-associate-class partially balanced designs. NBS Applied Mathematics Series 63, National Bureau of Standards, U. S. Department of Commerce.

- [3] Hedayat, A. and E. Seiden (1970). F-square and orthogonal F-squares design: A generalization of latin square and orthogonal latin squares design. Ann. Math. Statist. 41 2035-2044.
- [4] Joiner, J. R. (1973). Similarity of designs in fractional factorial experiments. Ph.D. Thesis, Cornell University, August.
- [5] Paik, U. B. and W. T. Federer (1970). A randomized procedure of saturated main effect fractional replicates. Ann. Math. Statist. 41 369-375.
- [6] Raktoe, B. L. and W. T. Federer (1970). A characterization of optimal saturated main effect plans of the 2^n factorial. Ann. Math. Statist. 41 203-206.
- [7] Srivastava, I. N., B. L. Raktoe, and H. Pesotan (1971). On invariance and randomization in fractional replication. (In the process of publication.) Department of Mathematics and Statistics, University of Guelph.